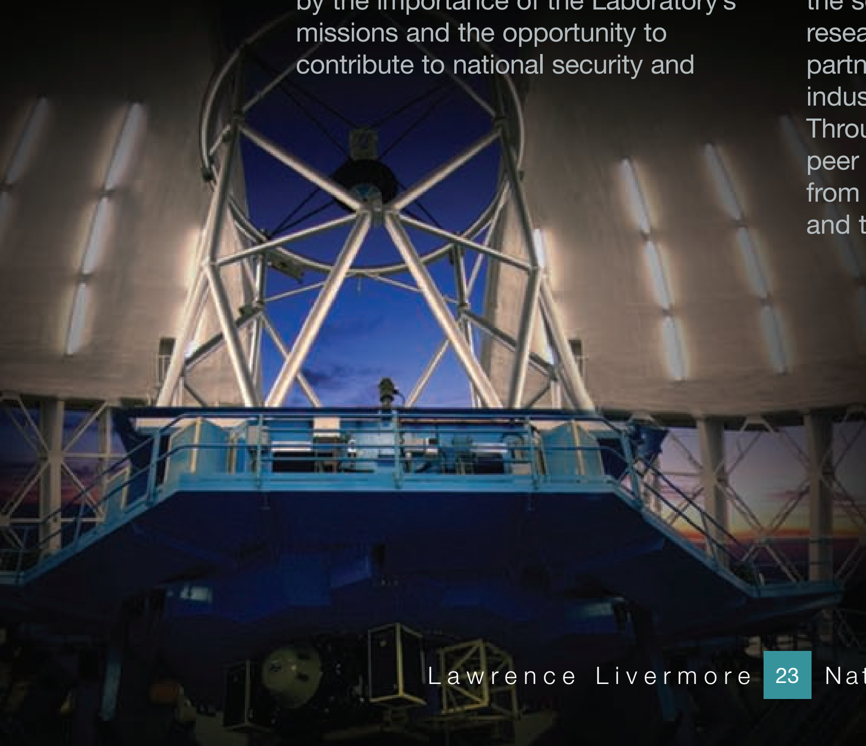
R&D Advances Laboratory Missions

Lawrence Livermore is a home of extraordinary science and technology. We are a place where researchers model the motion of millions of atoms for billionths of a second to determine the property of materials and also simulate weather patterns and ocean currents on the scale of tens of kilometers for hundreds of years to study climate change. Engineers develop micromechanical systems to quickly detect biological agents and search for planets in other solar systems. Scientists manufacture new materials by layering atoms to make, for example, mirrors for x rays that are used to image complex molecules. The particle is frozen in motion because the pulse of the x rays is only quadrillionths of a second long.

More than by the prospect of scientific discovery or technical breakthrough, our scientists and engineers are motivated by the importance of the Laboratory's missions and the opportunity to contribute to national security and global stability. We take a multidisciplinary approach to problem solving by drawing on the work of exceptional individuals and team efforts.

The sponsors of our work rely on and invest in our unique capabilities, the special skills of our researchers, and our broad science and technology base. Our internal investments—such as the Laboratory Directed Research and Development Program—closely align with our missions. We strive to make dramatic advances to meet mission objectives and prepare for emerging national needs.

Breakthroughs made by Laboratory scientists and engineers often have broad applicability. For example, developments in adaptive optics that made NIF possible also vastly improve the capabilities of groundbased telescopes and aid in the search for distant planets. Our research efforts frequently entail partnerships with other laboratories, industry, and research universities. Through these collaborations and peer review of our work, we benefit from advances in international science and technology to meet mission needs.



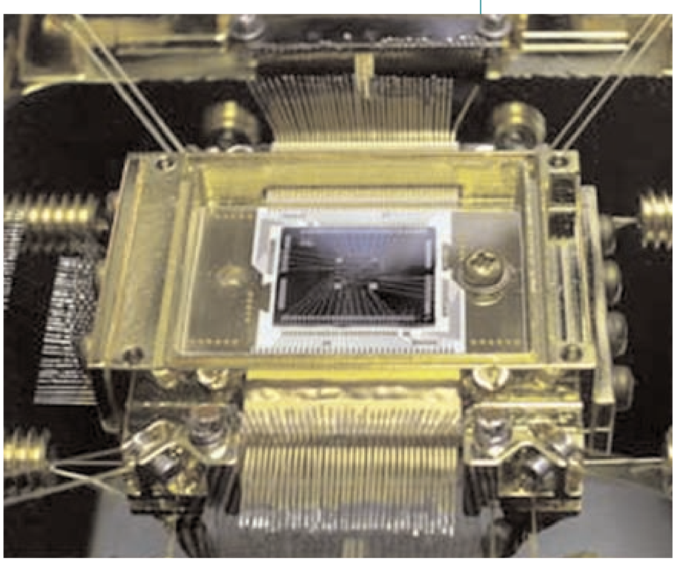
Cherry Murray
Principal Associate Director
Science and Technology

Materials at the Fundamental Level

Experiments performed at the FLASH free-electron laser facility in Hamburg, Germany, demonstrated a new technique for studying the dynamic properties of materials under extreme conditions. Sir Isaac Newton's "dusty mirror experiment" gave a Laboratory physicist the idea for the work, and results were reported in the August 9, 2007, issue of *Nature*. The research team placed an x-ray mirror a short distance behind the targeted material. An extremely short x-ray laser pulse blew up the target, and the pulse bounced off the mirror, allowing the researchers to look at the object again after it exploded. The diffracted light from the pulse and its reflection were combined, creating an interference pattern that was used to form a hologram (three-dimensional image) of the object at the scale of nanometers and femtoseconds (quadrillionths of a second). This technique was developed for experiments that will image single molecules using the Linac Coherent Light Source at Stanford University when it opens in 2009.

To probe the properties of materials under extreme static conditions, Laboratory researchers use a diamond anvil cell. One research team studied the electronic spin state of iron in ferropericlase (iron magnesium oxide) at the high temperatures and pressures that exist in Earth's lower mantle. They were able to determine the location of the spin-transition zone in the mantle, where iron is in a mixture of high- and low-spin states. Ferropericlase is the second most abundant mineral in the lower mantle, and by determining its spin state, scientists can better understand Earth's structure, composition, and dynamics, which affect geological activities on the planet's surface.

Researchers used this detector to obtain the most accurate measurements yet of the energy difference between the ground state and the first excited state (isomer) of thorium-229. This success brings scientists one step closer to being able to turn on and off the decay of a nuclear isomer.



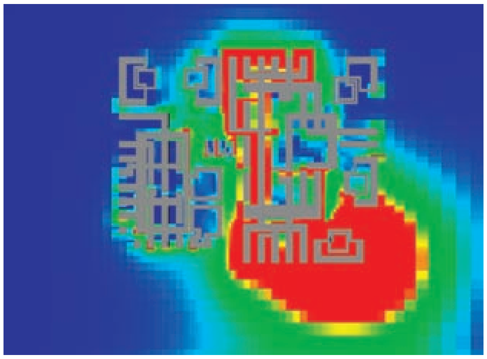
The April 6, 2007, issue of *Physical Review Letters* reported on the efforts of a Livermore-led nuclear physics collaboration that measured the energy difference between the ground and first excited (isomer) state of thorium-229. Excited states of nuclei are thousands of times more energetic than electron excited states. The thorium isomer is of particular interest because the energy difference is low enough that the isomer is accessible to laboratory study. The next step is to use a tabletop laser to transition thorium-229 nuclei between its ground and isomeric states. The amount of energy that could be stored would be much higher than that in conventional energy storage devices, opening up exciting potential applications and new physics to explore.

Supercomputing Challenges

In 2007, Livermore's "Grand Challenge" scientific computing program allocated 83.7 million hours of machine time on the Atlas and Thunder supercomputers to 17 research projects. Atlas and Thunder, at 44 teraflops and 23 teraflops, respectively, are the workhorses for unclassified, high-end computing across the Laboratory. To be considered for the program, a project has to address a grand-challenge-scale, mission-related problem that promises unprecedented discoveries in a particular scientific and/or engineering field of research. An additional criterion is that if the work is successful, it will result in high-level recognition by the scientific community at large. Results from calculations on the two machines advanced research in nuclear physics, materials science, global climate change, and more.

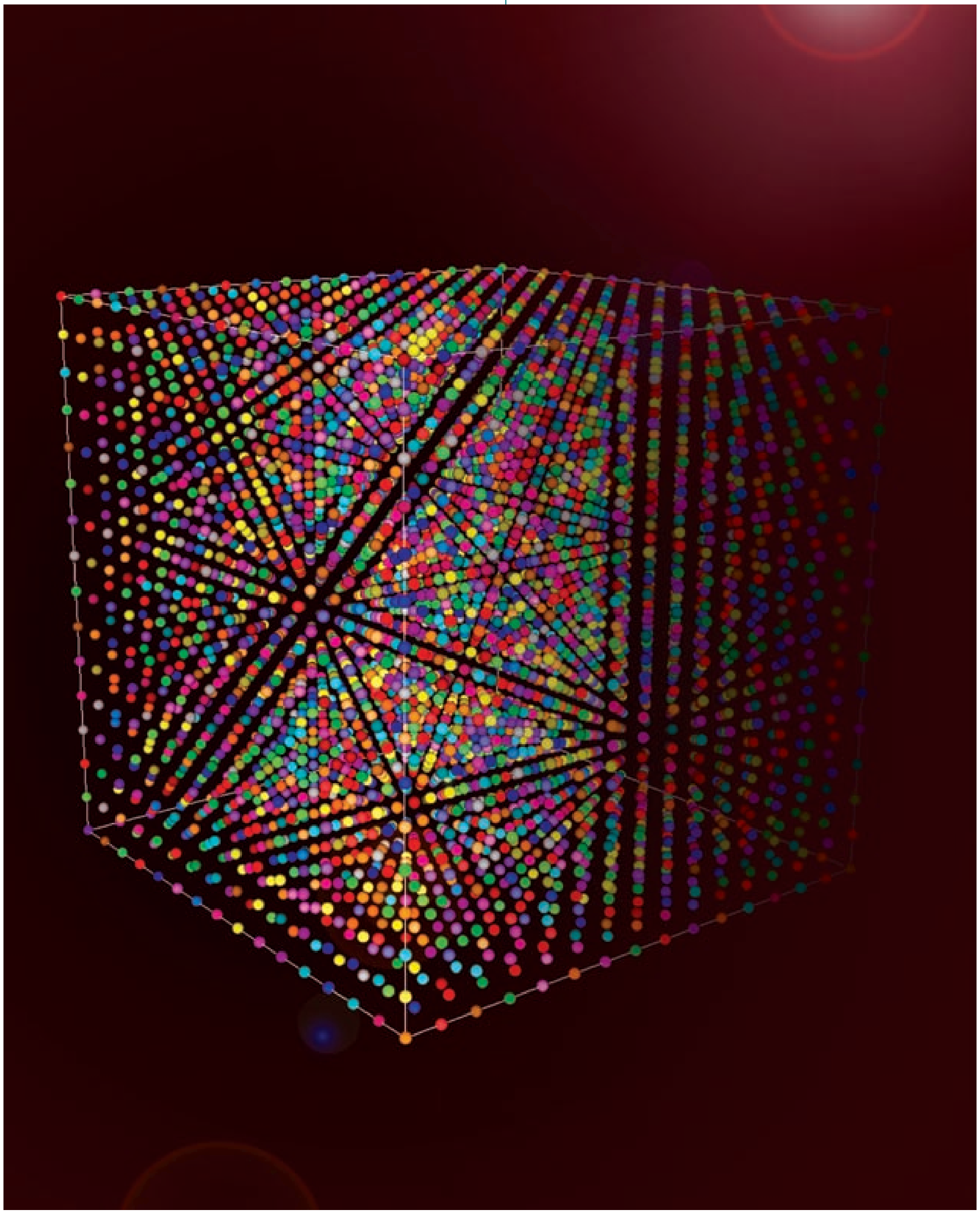
The March 2007 cover of *IEEE Transactions on Magnetics* featured simulations of magnetic fields in complex geometries using EMSolve, a computer code developed at Livermore for simulating the propagation and interaction of electro-magnetic fields. It is the most accurate, powerful, and flexible tool ever developed for solving Maxwell's equations, which describe how a changing magnetic field produces an electric field and vice versa. Laboratory scientists and engineers use EMSolve to simulate electromagnetic fields in structures ranging in size from a computer chip to a two-story building. Magnetic fusion energy, lasers, radar, nuclear weapons effects, electronics, and communication systems all involve electromagnetic phenomena that must be accurately calculated. EMSolve has also been licensed to private industry.

BlueGene/L, the world's most powerful computer (see p. 8), is proving to be an essential tool for studying the behavior of nuclear particles immediately after the big bang. Quarks, the building blocks of all nuclear material, ran free in a hot plasma for about 10 millionths of a second after the big bang. As the universe continued to expand and cool, the quarks coalesced into protons and neutrons. In a very brief reverse big bang, experiments at Brookhaven National Laboratory succeeded in creating individual quarks by colliding extremely high energy gold ions. The particle interactions were much stronger than expected. To explore the discrepancies, a large Livermore-led collaboration is simulating the plasma from when the transition from quarks to larger particles occurred to determine its equation of state. Only with an accurate equation of state can the full hydrodynamics of the transition be modeled. Equation-of-state calculations to date have narrowed the estimated temperature at the transition—approximately 2 trillion degrees or 170 million electronvolts—to within about 10 million electronvolts.



An analysis using the electromagnetic code EMSolve studied noise in integrated circuits containing both digital and analog components. In this simulation, red denotes the highest magnitude and blue the lowest of the electric current in the substrate.

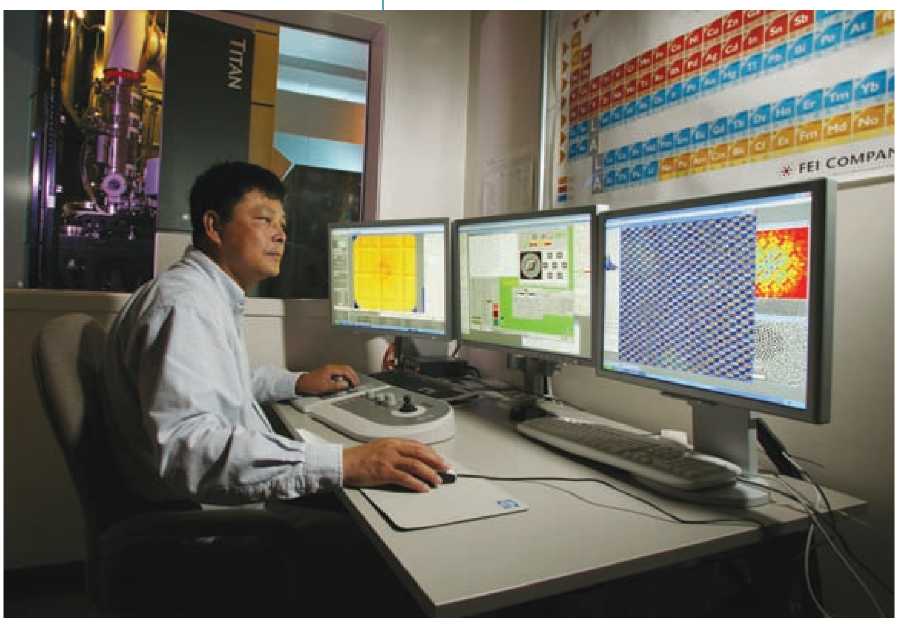
A simulation of quark behavior determines the potential energy between two quarks. Various types of quarks make up protons, neutrons, and other nuclear particles.

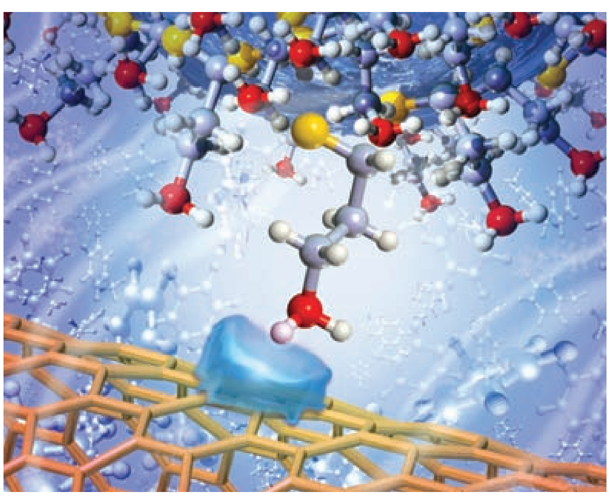


Tools to Power Nanoscale Research

Acquired in 2007, the Laboratory's new super scanning transmission electron microscope (SuperSTEM) is the highest resolution microscope in the world and is one of several new devices at the Laboratory that are revealing the behavior of materials at the formerly invisible nanometer scale (1 million nanometers equals 1 millimeter). This more advanced instrument, able to resolve features as small as 0.08 nanometers, replaces the world's first super scanning microscope, which was installed at the Laboratory in 2004 and used in the analysis of samples from Comet Wild 2. SuperSTEM is an advanced form of a transmission electron microscope with an added electron beam that focuses on a narrow area of the sample and scans it, providing the means to derive the identity and chemical and electronic states of individual atoms. This information is obtained simultaneously as an image builds up, thereby forming a direct correlation between the image and electronic data. SuperSTEM produces images magnified more than 1 million times.

The Laboratory's newest super scanning transmission electron microscope can resolve objects less than 1 angstrom.





An artist's rendering depicts an experiment that achieved a true single function group interaction. An amine functional group, attached to the tip of a probe, is brought near the surface of a carbon nanotube. As it approaches, a polarization charge, shown by the translucent blue shape, forms on the nanotube.

With chemical force microscopy—a nanoscale technique that measures interaction forces using tiny springlike sensors—researchers measured a single interaction of a chemical functional group with a carbon nanotube. Carbon nanotubes are used in composite materials, biosensors, nanoelectronic circuits, and membranes. Yet little is known about the interaction at the atomic scale of nanotubes and chemical functional groups, the smallest group of atoms that determines the chemical reactions of a molecule. Livermore scientists achieved a true single function group interaction by reducing the probe–nanotube contact area to about 1.3 nanometers. Their research, published in the October 14, 2007, online issue of *Nature Nanotechnology*, indicates that the interaction strength depends on the intricate electronic interactions between the nanotube and the functional group. Understanding these interactions is necessary for the engineering of future generations of sensors and nano devices that will rely on single-molecule coupling between components.

Using a high-resolution secondary ion mass spectrometer (NanoSIMS), a team that included Livermore researchers has shown that blue-green algae are significant species in the global carbon cycle. Imaging and tracking nutrient uptake at the nanoscale revealed that these cyanobacteria transform nitrogen gas from the atmosphere into a usable nutrient, enabling photosynthesis in nutrient-poor waters. NanoSIMS provided the ability to map the distributions of elements and isotopes with a 50- to 100-nanometer resolution. The research, which demonstrated the utility of NanoSIMS as a cellular microbiology research tool, appeared in the August 1, 2007, issue of *The International Society for Microbial Ecology Journal*.

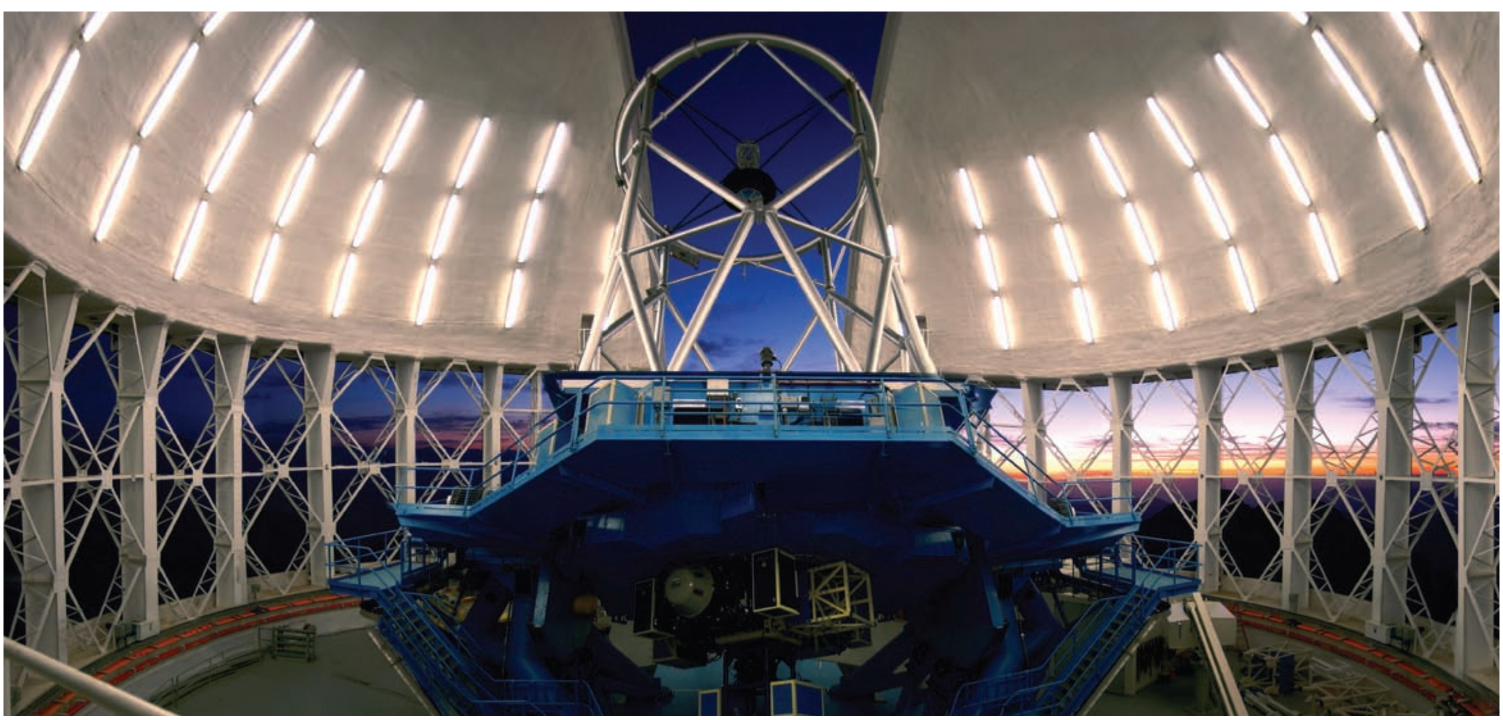
Sharp Focus on Adaptive Optics

Livermore leads an international consortium that is developing the Gemini Planet Imager, which will allow scientists to directly image planets around distant stars. When it comes online in Chile in 2010, the Imager will bring into sharp focus planets and other objects 30 to 150 light years from our solar system. It will be the most capable adaptive optics system in the world.

Adaptive optics use a mirror whose shape can be adjusted hundreds of times per second. This allows astronomers to compensate for atmospheric turbulence and take the twinkle out of starlight, bringing into focus stars, galaxies, and planets in a telescope's field of view. At the heart of the Gemini Planet Imager are next-generation adaptive optics designed by Laboratory scientists to gain even sharper, higher-contrast images. To keep the mirror small while incorporating 10 times as many actuators as in current adaptable mirrors, scientists chose a silicon microelectro-mechanical system (MEMS) device. It is lithographically patterned and etched like a microchip. The Laboratory is home to one of the world's best adaptive optics teams, which apply the technology to the National Ignition Facility, satellite-based surveillance, astronomy, vision correction, and more.

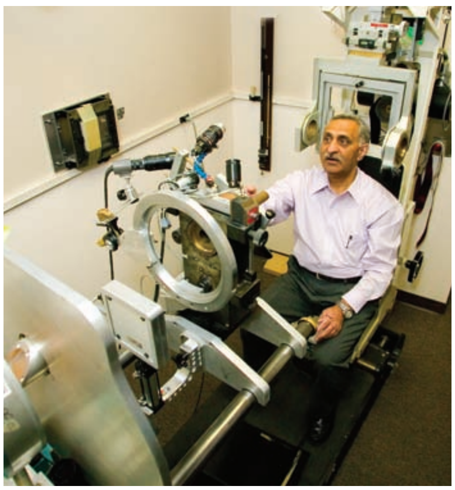
Livermore physicists used adaptive optics to discover the location and makeup of a pair of supermassive black holes at the center of a collision of two galaxies more than 300 million light years away. Scientists at the W. M. Keck Observatory in Hawaii were able to obtain clear images of the hot dust in the infrared wavelength, the stars in the visible and infrared, and the x rays and radio emissions coming from around the black holes. These observations lend support to the theory that black holes at the center of galaxies reach their immense mass through mergers with nearby black holes. Studying galaxy mergers is a way to learn how galaxies evolve and the role black holes play in the process.

A MEMS-based adaptive optics system is central to a new ophthalmoscope that won a Laboratory team an R&D 100 Award in 2007. The ophthalmoscope sharpens images of the retinal cell layers in a patient's eye, allowing clinicians to diagnose macular degeneration and other retinal diseases much earlier than was previously possible. The system can also be used to monitor a patient's treatment. Similarly, a team from national laboratories, universities, and private industry has developed a miniscule device that is inserted in the human eye to restore some sight for those with retinal disease. Livermore engineers designed the MEMS-based array of actuators.



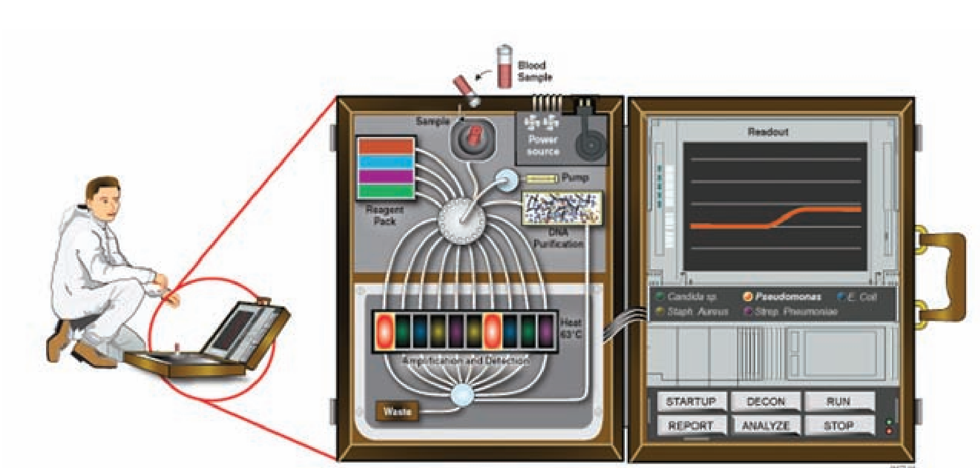
The Gemini Planet Imager, which will allow scientists to directly image planets around distant solar systems, will be installed at the Gemini South telescope in Chile in 2010. (Courtesy of Gemini Observatory and the Association of Universities for Research in Astronomy.)

A medical physicist at the University of California (UC) at San Francisco shows how a patient with melanoma of the eye would receive proton beam therapy when a proposed compact proton therapy machine is available. Here he uses a larger device at the Crocker Nuclear Laboratory at UC Davis, which is partnering with Livermore in developing the new device.



Improving Human Health

TomoTherapy Incorporated of Madison, Wisconsin, entered into an agreement with the Laboratory and UC Davis in June to develop the first compact proton therapy system, one that will fit in any major cancer center and cost a fifth as much as the larger machines used today. Proton therapy is considered the most advanced form of radiation therapy available, but size and cost have limited the technology's use to only six cancer centers nationwide. TomoTherapy is funding development of the first clinical prototype, which will be tested on patients by physicians at the UC Davis Cancer Center. Livermore researchers overcame the size obstacle by using a dielectric wall accelerator developed through defense research. They have demonstrated in principle that this technology will accelerate proton particles to an energy of at least 200 million electronvolts within a light-weight, insulator-based structure just 2.2 meters long. Existing systems use accelerators that weigh up to several hundred tons and are the size of a basketball court. The new system will also improve on existing technology by including the capability to vary the energy, intensity, and "spot" size of the proton beam.



This artist's illustration depicts how the point-of-care diagnostic unit being developed by Livermore and the University of California at Davis will operate. Doctors will be able to identify bloodstream infections in an hour instead of a day or more.

Researchers from the Laboratory and the UC Davis Health System were awarded a five-year grant in November 2007 to develop new technologies for "point-of-care" (POC) testing. Instead of having to transport a blood sample to a hospital, doctors will be able to diagnose bloodstream infections at the scene of a disaster. The National Institute of Biomedical Imaging and Bioengineering, part of the National Institutes of Health, granted funds to develop two prototype instruments that simultaneously conduct five bacterial and fungal evaluations. One instrument is for use in hospital settings and the other is portable, for use in the field. Grant funds will also be used to evaluate other exploratory diagnostic technologies intended to prepare the nation for disasters. This work is being undertaken through the UC Davis–Livermore Center for POC Technologies, which is part of the newly established National Institute of Biomedical Imaging and Bioengineering POC Technologies Research Network.

A Livermore team has developed a new method using accelerator mass spectrometry (AMS) to examine the metabolism of a chemical DNA lesion called 8-oxodG, one of the most prevalent mutagenic lesions found in DNA and an apparent cause of cancers and diseases related to aging. Their findings were featured on the cover of the July 3, 2007, issue of the *Proceedings of the National Academy of Sciences*. Considerable data exist about how DNA can repair this lesion, but little was known about where in the cell 8-oxoG is formed and how it is metabolized and incorporated into DNA. With AMS, the team precisely measured the metabolism of 8-oxoG in a type of human breast cancer cell called MCF-7. Researchers exposed cells to 8-oxoG tagged with carbon-14 and used AMS to measure the incorporation of 8-oxoG into MCF-7 cells over time. This research demonstrated that 8-oxoG can be absorbed by the cells and incorporated in the DNA to cause mutations that lead to disease. Prior to this study, researchers believed that 8-oxodG only formed directly in the DNA.